Novel Monte Carlo study of deposited magnetic nanoparticles

L. Balogh[1], K. M. Lebecki[2], B. Lazarovits[3], L. Udvardi[1], L. Szunyogh[1], U. Nowak[2]

[1] Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1111 Budapest, Hungary

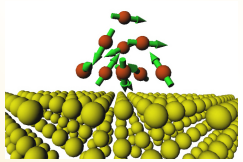
[2] Fachbereich Physik, Universität Konstanz, D-78464 Konstanz, Germany

[3] Research Institute for Solid State Physics and Optics, HAS, Konkoly-Thege Miklós út 29-33, Budapest, Hungary

E-mail: udvardi@phy.bme.hu

Introduction

- In order to study the finite temperature behavior of magnetic nanoparticles, a novel Monte Carlo method has been developed. The energy of a new trial configuration during the simulation is calculated directly from the expansion of the band energy avoiding the set up of an *a priori* Heisenberg-type model.
- Studies of deposited magnetic nanoparticles



magnetic cluster, e.g., Cr, Co

non-magnetic (semi-infinite) host, e.g., Au(111), Cu(001)

- The magnetic properties of a wide class of systems are often described by the classical Heisenberg model,

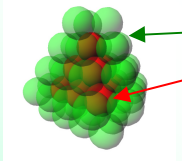
$$\mathcal{H} = \frac{1}{2}\sum_{i,j} J_{ij}\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j - \sum_i K\,(\boldsymbol{\sigma}_i^z)^2,$$

where isotropic coupling between spins and uniaxial anisotropy are considered. We compare the *ab initio* and the Heisenberg model based temperature dependence of the magnetic moment of a Co_{4x4}|Cu(001) cluster, and find good agreement for this particular case.

Computational method I. – Electronic structure

- Electronic structure calculation: fully relativistic implementation of the local spin-density approximation of the density functional theory
- Embedded cluster Green's function technique based on the KKR method [1]

$$\boldsymbol{\tau}(\varepsilon) = \boldsymbol{\tau}_{\mathrm{host}}(\varepsilon)\left(\mathbf{I} - \Delta\mathbf{t}^{-1}(\varepsilon)\boldsymbol{\tau}_{\mathrm{host}}(\varepsilon)\right)^{-1}$$



environment (vacuum or host atoms)

real cluster (e.g., Cr or Co atoms)

} cluster

- Self-consistent cluster calculation
- then: frozen potential approximation

- Taylor-expansion of the band energy:

$$E_b \approx E_0 + \sum_{i=1}^{N}\left.\frac{\partial E_b}{\partial\boldsymbol{\sigma}_i}\right|_{\{\boldsymbol{\sigma}_0\}}\Delta\boldsymbol{\sigma}_i + \frac{1}{2}\sum_{i,j=1}^{N}\Delta\boldsymbol{\sigma}_i^{\mathrm{T}}\left.\frac{\partial^2 E_b}{\partial\boldsymbol{\sigma}_i\partial\boldsymbol{\sigma}_j}\right|_{\{\boldsymbol{\sigma}_0\}}\Delta\boldsymbol{\sigma}_j$$

- The derivatives of the band energy can be calculated analytically from Lloyd's formula, see [2].

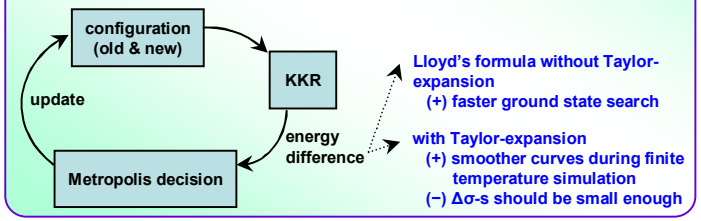
$$E_b = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\varepsilon_F}\mathrm{Tr}\ln\boldsymbol{\tau}(\varepsilon)\,\mathrm{d}\varepsilon$$

Computational method II. – Monte Carlo simulation

- Ground state by simulated annealing
- Finite temperature simulation
- We used the Metropolis algorithm with single spin flip dynamics:

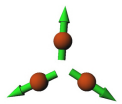
$$P(i\to f) = \begin{cases} 1, & \text{if } E_f \le E_i, \\ e^{-\beta(E_f - E_i)}, & \text{if } E_f > E_i. \end{cases}$$

- Flowchart of the code:



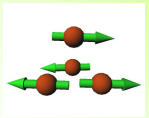
Results I. – Ground state of AFM and FM clusters

- Benchmark system: Cr trimer on Au(111) surface. The same ground state was found in [3] by solving the Landau–Lifshitz–Gilbert equations.



frustration ⇩ non-collinear ground state

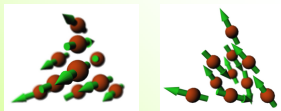
- Tetrahedron shaped Cr particle on Au(111) surface. Similar ground state was found in [4] for the same Cr cluster on Cu(111) surface.



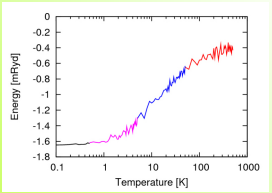
collinear ground state

- Ground state of a pyramid shaped Cr_{10} cluster on Au(111) surface

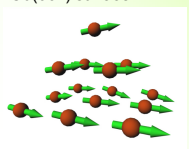
(top view) (side view)



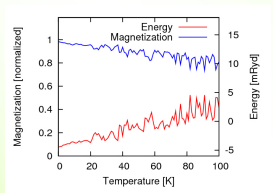
- Simulated annealing of this cluster in four steps



- Ground state of a pyramid shaped Co_{14} cluster on Cu(001) surface

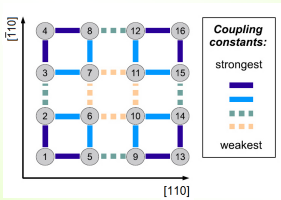


- Simulated annealing of this cluster



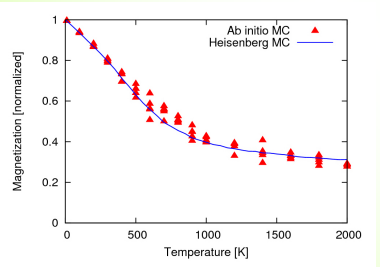
Results II. – Thermodynamics of a Co_{4x4}|Cu(001) cluster

- Geometry and isotropic coupling constants between next nearest neighbors



Coupling constants	[mRyd]	Magnetic moments	[μ_B]
J_{1-5}	5.59	m_1	1.74
J_{5-6}	5.27	m_5	1.82
J_{5-9}	4.49	m_6	1.87
J_{6-10}	4.19		
$J_{\mathrm{mono\text{-}layer}}$	4.26	$m_{\mathrm{mono\text{-}layer}}$	1.88

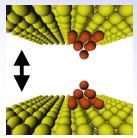
- Square root of the thermal average of the square of the magnetization:



➢ In the Heisenberg MC simulation, we used 10^5 MC steps per temperature points and the anisotropy constant of the monolayer cobalt on Cu(001) surface, K = 0.0228 mRyd;
➢ in the *ab initio* MC simulation we used 5 x 10^4 MC steps per temperature points.

Future plans

- Simulating an "STM tip" and investigating the distance-dependence of its magnetic structure and ground state
- Further studies of the thermodynamics of magnetic nanoparticles (magnetic switching)



References and acknowledgments

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